A COMPREHENSIVE MODEL OF SUBCRITICAL AND SUPERCRITICAL DROP EVAPORATION STARTING FROM FIRST PRINCIPLES

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Abstract

A model describing the behavior of a fluid oxygen drop in a fluid hydrogen environment at arbitrary pressure and temperature has been developed starting from basic physical principles in order to provide generally applicable equations. This approach enables systematic and known approximations to be made, as necessary.

Mixture properties may be described either by using thermodynamic activity coefficients, or equivalently, by an equation of state. In either case, a semi-empirical approach is needed, as neither theory nor experiment by themselves provide adequate means of mixture description. This approach is the standard description of thermodynamic mixture properties outside the range of ideal gas behavior. Transport of mass and energy is proportional to gradients of the thermodynamic variables pressure, temperature and mole fraction (or mass fraction). For generalized nonequilibrium processes, this approach is validated by use of statistical calculations of molecular level interactions known as fluctuation theory. The transport equations combine with conservation equations for mass, momentum and enthalpy to form the model.

An important aspect of the model is that it is not necessary to assume that there is a surface at the boundary between the "blobs" or "pseudo-drops" of oxygen and the hydrogen. Similarly, it is not necessary to assume that oxygen is in liquid phase. It is the

solution for the density which indicates whether oxygen is in the liquid phase or if it is a heavy gas (a fluid).

The drop model is a non steady, spherically symmetric model wherein far field pressure, temperature and mole fraction are prescribed functions of time. For subcritical conditions, nonequilibrium thermodynamics describes evaporation at the drop surface. For the supercritical case, the boundary of the high concentration oxygen region is one of solvation (or mixing) with conventional evaporation absent.

The model requires values of various transport coefficients and thermodynamic parameters describing mixture properties. For oxygen-hydrogen mixtures, there is a shortage of information needed for a complete, accurate model formulation. Parametric studies will be needed to determine the sensitivity of the model to those values ill-defined.

Conditions for hydrogen will be supercritical relative to its pure state, Conditions for oxygen may be subcritical or supercritical (and may change during a calculation). In the former case, a phase distinction (gas-liquid) can exist with corresponding surface tension, or energy, at phase boundaries leading to stable drop formation. For the latter case, the mixture as a whole is expected to exist as a nondistinct fluid phase where the usual concept of drops does not apply. However, a pseudo-drop model, as discussed above, may be used to describe regions of high oxygen concentration (e.g., irregular oxygen blobs or regular oxygen rich small scale vortex structures).

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